Benzamide, N-ethyl-N-(3-methylphenyl)-3-methoxy-

Inchi: InChI=1S/C17H19NO2/c1-4-18(15-9-5-7-13(2)11-15)17(19)14-8-6-10-16(12-14)20-3/h5-1

InchiKey: WQNZNISNAJJSRF-UHFFFAOYSA-N

Formula: C17H19NO2

SMILES: CCN(C(=O)c1cccc(OC)c1)c1cccc(C)c1

Mol. weight [g/mol]: 269.34

Physical Properties

Property code	Value	Unit	Source
gf	174.68	kJ/mol	Joback Method
hf	-121.36	kJ/mol	Joback Method
hfus	32.90	kJ/mol	Joback Method
hvap	70.51	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.670		Crippen Method
mcvol	220.290	ml/mol	McGowan Method
pc	2115.83	kPa	Joback Method
rinpol	2062.00		NIST Webbook
rinpol	2062.00		NIST Webbook
tb	740.41	K	Joback Method
tc	967.39	K	Joback Method
tf	463.86	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.33	J/mol×K	740.41	Joback Method
cpg	626.53	J/mol×K	778.24	Joback Method
cpg	641.52	J/mol×K	816.07	Joback Method
cpg	655.34	J/mol×K	853.90	Joback Method
cpg	668.05	J/mol×K	891.73	Joback Method
cpg	679.71	J/mol×K	929.56	Joback Method
cpg	690.37	J/mol×K	967.39	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308148&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume